

Phase separation and vortex states in binary mixture of Bose-Einstein condensates in the trapping potentials with displaced centers

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(Dated: 24 January 2002)

The system of two simultaneously trapped condensates consisting of ^{87}Rb atoms in two different hyperfine states is investigated theoretically in the case when the minima of the trapping potentials are displaced with respect to each other. It is shown that the small shift of the minima of the trapping potentials leads to the considerable displacement of the centers of mass of the condensates, in agreement with the experiment. It is also shown that the critical angular velocities of the vortex states of the system drastically depend on the shift and the relative number of particles in the condensates, and there is a possibility to exchange the vortex states between condensates by shifting the centers of the trapping potentials.

PACS numbers: 03.75.Fi, 67.57.Fg, 67.90.+z

The experimental realization of Bose-Einstein Condensation (BEC) in trapped alkali-atoms gases at ultralow temperatures offers new opportunities for studying quantum degenerate fluids [1, 2, 3]. The art of manipulating these condensates, which contain thousands of atoms confined to microscale clouds, achieved very high level now. Creation of vortices in one [4] and two-component BEC [5, 6] of ^{87}Rb atoms is the amazing example of this art.

In this article we focus on the properties of the two-component BEC in the trap in which the trapping potentials for each component are displaced with respect to each other in the vertical direction [7]. The condensate consists of the simultaneously trapped otherwise identical atoms of ^{87}Rb in two different hyperfine spin states $|1\rangle$ and $|2\rangle$ ($|1\rangle$ and $|2\rangle$ denote the $|F=1, m_f=-1\rangle$ and $|2, 1\rangle$ spin states of ^{87}Rb atoms respectively) [7, 8, 9]. The scattering lengths of the states $|1\rangle$ and $|2\rangle$ are known to be in proportion $a_{11} : a_{12} : a_{22} = 1.03 : 1.0 : 0.97$ with the average of the three being $55(3)\text{\AA}$ [7, 8, 9].

The double condensate system was prepared from the single $|1\rangle$ condensate by driving a two-photon transition which transfers any desired fraction of the atoms to the $|2\rangle$ state by selecting the length and amplitude of the two-photon pulse [8]. The rotating magnetic field of the time-averaged orbiting potential (TOP) trap gave the possibility to displace the minima of the trapping potentials V_1 and V_2 with respect to each other. When the minima of the trapping potentials were not shifted, the $|1\rangle$ atoms formed a shell about the $|2\rangle$ atoms [7]. This case has been discussed theoretically in [10, 11]. If the minima of the trapping potentials V_1 and V_2 are displaced from each other by a distance which is small compared to the size of the total condensate the resulting separation of the centers of mass of the condensates is much larger

[7]. In this paper we provide for an analytical explanation of this result.

In order to explore the boundary between the two condensates, we begin with the analysis of their behaviour in the framework of the Thomas-Fermi Approximation (TFA), which ignores the kinetic energy terms in the Gross-Pitaevskii equations for the condensate wave functions [12]. It has been shown that in the case of one component condensates the TFA results agree well with the numerical calculations for large particle numbers, except for a small region near the boundary of the condensate [13, 14]. In fact, even for small numbers of particles TFA still usually gives qualitatively correct results.

In the dimensionless variables, the Gross-Pitaevskii equations for the condensates in the harmonic traps may be written in the form [10, 11]:

$$-\nabla'^2\psi'_1 + (x'^2 + y'^2 + \lambda^2(z' + z'_0)^2)\psi'_1 - \mu'_1\psi'_1 + u_1|\psi'_1|^2\psi'_1 + \frac{8\pi a_{12}N_2}{a_\perp}|\psi'_2|^2\psi'_1 = 0; \quad (1)$$

$$-\beta^2\nabla'^2\psi'_2 + (x'^2 + y'^2 + \lambda^2(z' - z'_0)^2)\psi'_2 - \mu'_2\psi'_2 + u_2\beta^2|\psi'_2|^2\psi'_2 + \frac{8\pi a_{12}N_1}{a_\perp}|\psi'_1|^2\psi'_2 = 0; \quad (2)$$

Here $\psi_i(\mathbf{r}) = \sqrt{N_i/a_\perp^3}\psi'_i(\mathbf{r}')$, $\psi_i(\mathbf{r})$ being the wave function of the species i of a two-species condensate ($i = 1, 2$). $\lambda = \omega_z/\omega$. $\mathbf{r} = a_\perp\mathbf{r}'$, where $a_\perp = (\hbar/m\omega)^{1/2}$. ω is the trapping frequency. $\mu'_i = 2\mu_i/\hbar\omega$, where μ_i is the chemical potential of the species i . The chemical potentials μ_1 and μ_2 are determined by the relations $\int d^3|\psi_i|^2 = N_i$. u_i is given by $u_i = 8\pi a_{ii}N_i/a_\perp$. The wave function $\psi'_i(\mathbf{r}')$ is normalized to 1. z'_0 denotes the shift of the minimum of the trapping potential in the vertical direction.

Equations (1) and (2) were obtained by minimization

of the energy functional of the trapped bosons given by:

$$\begin{aligned}
E' = & \frac{1}{2} \int d^3 r' [N_1 |\nabla' \psi'_1|^2 + N_2 \beta^2 |\nabla' \psi'_2|^2 + \\
& + N_1 (x'^2 + y'^2 + \lambda^2 (z' + z'_0)^2) |\psi'_1|^2 + \frac{1}{2} N_1 u_1 |\psi'_1|^4 + \\
& + N_2 (x'^2 + y'^2 + \lambda^2 (z' - z'_0)^2) |\psi'_2|^2 + \\
& + \frac{1}{2} N_2 u_2 \beta^2 |\psi'_2|^4 + \frac{4\pi a_{12}}{a_\perp} N_1 N_2 |\psi'_1|^2 |\psi'_2|^2] . \quad (3)
\end{aligned}$$

Here the energy of the system E is related to E' by $E = \hbar\omega E'$

In the TFA, Eqs. (1), (2) and (3) can be further simplified by omitting the kinetic energy terms. In the framework of TFA the phase segregated condensates do not overlap, so we can neglect the last terms in Eqs. (1), (2) and (3), obtaining simple algebraic equations:

$$\begin{aligned}
|\psi'_1(\mathbf{r}')|^2 = & \frac{1}{u_1} \left(\mu'_1 - (r'^2 + \lambda^2 (z' + z'_0)^2) \right) \times \\
& \times \Theta \left(\mu'_1 - (r'^2 + \lambda^2 (z' + z'_0)^2) \right) \times \\
& \times \Theta \left(r'^2 + \lambda^2 (z' - z'_0)^2 - \mu'_2 \right); \quad (4)
\end{aligned}$$

$$\begin{aligned}
|\psi'_2(\mathbf{r}')|^2 = & \frac{1}{u_2} \left(\mu'_2 - (r'^2 + \lambda^2 (z' - z'_0)^2) \right) \times \\
& \times \Theta \left(\mu'_2 - (r'^2 + \lambda^2 (z' - z'_0)^2) \right) \times \\
& \times \Theta \left(r'^2 + \lambda^2 (z' + z'_0)^2 - \mu'_1 \right). \quad (5)
\end{aligned}$$

Here Θ denotes the unit step function and $\rho'^2 = x'^2 + y'^2$. If $z'_0 = 0$, from Eqs. (4) and (5) one can see that the condensate density has the ellipsoidal form. This case has been considered in detail in Refs. [10, 11].

In the case of phase separation, the energy of the system can be written in the form [10, 11] $E = E_1 + E_2$, where

$$E_1 = \frac{1}{2} \hbar\omega N_1 \left[\mu'_1 - \frac{1}{2} u_1 \int d^3 r' |\psi'_1|^4 \right], \quad (6)$$

$$E_2 = \frac{1}{2} \hbar\omega N_2 \left[\mu'_2 - \frac{1}{2} u_2 \int d^3 r' |\psi'_2|^4 \right]. \quad (7)$$

To determine the position of the boundary between the condensates, we use the condition of thermodynamic equilibrium [15]: the pressures exerted by both condensates must be equal: $P_1 = P_2$. Pressure is given by [16]: $P_i = G_{ii} |\psi_i|^4 / 2$, where $G_{ii} = 4\pi \hbar^2 a_{ii} / m_i$. Using these equations one can obtain the equation for the phase boundary:

$$r''^2 + \left(\lambda z'' - \frac{\alpha(\kappa + 1)}{\kappa - 1} \right)^2 = R^2, \quad (8)$$

where $z' = \sqrt{\mu'_1} z''$, $r' = \sqrt{\mu'_1} r''$, $r'^2 = x'^2 + y'^2$, $\alpha = \lambda z''_0$, $\kappa = \sqrt{a_{11}/a_{22}}$, and

$$R^2 = \frac{\mu'_1 - \kappa \mu'_2}{\mu'_1 (1 - \kappa)} + \frac{4\alpha^2 \kappa}{(\kappa - 1)^2}. \quad (9)$$

From Eqs. (8) and (9) one can easily understand why the small displacement of the centers of the trapping potentials leads to the significant resulting separation of the centers of mass of the condensates [7]. The basic physics of this amplification of the trap center difference comes from the two possible final configurations of the mixture and that the system is **close** to the “critical point” that separates the two final configurations. The two configurations are the symmetric one where one component is inside and the other component is outside and the asymmetric one [17, 18, 19] where the two components are on opposite sides. The former configuration is favored when $\kappa = \sqrt{a_{11}/a_{22}}$ is different from one, with the less repulsive component in the middle where the density is higher. The asymmetric configuration possess a lower interface energy and is favored when κ is close to one. We found that in the Thomas-Fermi approximation, when the trapping frequencies for the two components are the same, the amplification factor is proportional to $1/(\kappa - 1)$.

From Eqs. (8)-(9) the evolution of the system upon increasing α may be described as follows: for $\alpha = 0$ condensate 1 forms the shell about the ellipsoidal condensate 2. The semiaxis of this ellipsoid is given by Eq. (8) for $\alpha = 0$. Upon increasing α the inner ellipsoid moves upwards, while external one moves down. It may be shown that they touch each other for the critical value of α : $\alpha_c = \frac{1}{2} \left(1 - \sqrt{\frac{\mu'_2}{\mu'_1}} \right)$. For $\alpha > \alpha_c$ phase boundary (8) intersect boundaries of condensates at the points with coordinates:

$$\lambda z''_c = \frac{\alpha}{\kappa - 1} - \frac{(\kappa - 1)(R^2 - 1)}{4\alpha\kappa}, \quad (10)$$

$$r''_{1,2} = \pm \sqrt{1 - (\lambda z''_c + \alpha)^2}, \quad (11)$$

which can be obtained from Eqs. (4)-(8). Critical value α_c is a function of the ratio N_2/N_1 .

Using normalization condition $\int |\psi'_i(\mathbf{r}')|^2 d^3 r' = 1$, one can determine the chemical potentials μ'_i as functions of N_1 , N_2 , and α . Analytical expressions for μ'_i are different for $\alpha < \alpha_c$ and for $\alpha > \alpha_c$. In the former case one has:

$$\frac{(\mu'_1)^{(5/2)}}{(\mu'_1)^{(5/2)}} = \frac{1}{1 - \frac{5}{2} R^3 [1 - \gamma^2] + \frac{3}{2} R^5}, \quad (12)$$

$$\frac{(\mu'_1)^{(5/2)}}{(\mu'_2)^{(5/2)}} = \frac{2}{15} \frac{1}{\frac{R^3}{3} [\frac{\mu'_2}{\mu'_1} - \tilde{\kappa}^2] - \frac{R^5}{5}}, \quad (13)$$

where $\mu'_i = \left(\frac{15\lambda u_i}{8\pi} \right)^{2/5}$, $\gamma = \frac{2\alpha\kappa}{\kappa-1}$, $\tilde{\kappa} = \gamma/\kappa$. In the limit $\alpha \rightarrow 0$ one has the results obtained in our previous papers for the non-displaced potential [10, 11]. In the case $\alpha > \alpha_c$ the formulas for μ'_1 and μ'_2 obtained after tedious but straightforward calculations are rather cumbersome and will be given elsewhere. In this article we discuss the results of calculations. To be specific, we will use the parameters corresponding to the experiments on ^{87}Rb atoms $a_\perp = 2.4 \times 10^{-4} \text{ cm}$, $N = N_1 + N_2 = 0.5 \times 10^6$ atoms, $\lambda = \sqrt{8}$.

In Fig.1 we show the density profiles of the condensates (see Eqs. (4) and (5)) as functions of the vertical coordinate z for $r'^2 = 0$ and $N_1 = N_2$. In this case $\alpha_c = 0.0047$. Fig.1(a) illustrates the experimental situation [7]: $\alpha = 0.03$ (approximately 3% of the extent of the density distribution in the vertical direction) is larger than the critical value α_c , and condensates are completely separated in vertical direction in accordance with the experiment [7]. In the case $\alpha < \alpha_c$ the condensate N_2 is inside the condensate N_1 . It should be noted that rather small shifts of the trapping potential centers with respect to each other produce considerable displacements of the condensates. The condensates in Fig.1 does not overlap because, as was mentioned earlier, in the framework of TFA it is impossible to describe the overlapping of the condensates.

Another interesting question is how the vortex states change when the minima of the trapping potentials V_1 and V_2 are displaced with respect to each other. In a frame rotating with the angular velocity Ω along the z -axis the energy functional of the system is:

$$E_{rot}(l_1, l_2) = E(\psi_{l_1}, \psi_{l_2}) + \int d^3r (\psi_{l_1}^* + \psi_{l_2}^*) i \hbar \Omega \partial_\phi (\psi_{l_1} + \psi_{l_2}) \quad (14)$$

where $\psi_{l_j}(\mathbf{r}) = |\psi_{l_j}(\mathbf{r})| e^{i l_j \phi}$ is the wave function for the vortex excitation with angular momentum $\hbar l_j$. In the TFA, the vortex induced change in condensate density is negligible [20] (hydrodynamic approximation).

In the case of the phase segregated condensate, one finds from Eqs. (14) and (6-7) that the energy change due to presence of the vortices $\Delta E = E_{rot}(l_1, l_2) - E_{rot}(0, 0)$ has the form [10, 11]:

$$\begin{aligned} \Delta E &= \Delta E_{N_1} + \Delta E_{N_2} = \\ &= \frac{1}{2} \hbar \omega N_1 \int d^3r' \left(\frac{l_1^2}{\rho'^2} |\psi'_1|^2 - \frac{2\Omega l_1}{\omega} |\psi'_1|^2 \right) + \\ &+ \frac{1}{2} \hbar \omega N_2 \int d^3r' \left(\frac{l_2^2}{\rho'^2} |\psi'_2|^2 - \frac{2\Omega l_2}{\omega} |\psi'_2|^2 \right). \end{aligned} \quad (15)$$

In the hydrodynamic limit ψ'_i is given by Eqs. (4) and (5).

In the case $\alpha = 0$ critical velocities as functions of ratio N_2/N_1 have been calculated in [10]. It was shown that for all values of N_2/N_1 , the critical velocity Ω_{N_2} of the inner condensate is lower than the critical velocity Ω_{N_1} of the outer one. So upon increasing Ω , a vortex will appear first in the external condensate. However, if for given Ω one shifts the centers of the trapping potentials

with respect to each other in the vertical direction, the inner condensate floats to the surface. In this case one can expect that the critical velocities of the condensates become closer and even can be equal for some values of α and N_2/N_1 .

As in the case of the chemical potentials, the expressions for the critical velocities have different analytical forms for $\alpha < \alpha_c$ and for $\alpha > \alpha_c$, the latter being rather cumbersome. For $\alpha < \alpha_c$ the critical velocities are given by:

$$\begin{aligned} \frac{\Omega_{N_1}}{\omega} &= \frac{5l_1(\mu'_1)^{(3/2)}}{2(\mu'_1)^{(5/2)}} \left\{ \left(\ln \frac{2\mu'_1}{l_1} - \frac{4}{3} \right) - \right. \\ &- \frac{3}{2} R \left[\left(1 - \gamma^2 - \frac{R^2}{3} \right) \ln \frac{2R\mu'_1}{l_1} - \right. \\ &- \left. \left(1 - \gamma^2 - \frac{R^2}{9} \right) \right] \left. \right\}, \end{aligned} \quad (16)$$

$$\begin{aligned} \frac{\Omega_{N_2}}{\omega} &= \frac{15l_2(\mu'_1)^{(3/2)}R}{4(\mu'_2)^{(5/2)}} \left[\left(\frac{\mu'_2}{\mu'_1} - \tilde{\kappa}^2 - \frac{R^2}{3} \right) \times \right. \\ &\times \left. \ln \frac{2R\sqrt{\mu'_1\mu'_2}}{l_2} - \left(\frac{\mu'_2}{\mu'_1} - \tilde{\kappa}^2 - \frac{R^2}{9} \right) \right]. \end{aligned} \quad (17)$$

Again, in the limit $\alpha \rightarrow 0$ one has the results obtained in our previous paper for the non-displaced potential [10].

Figure 2 shows the behaviour of critical velocities as functions of α for different values of N_2/N_1 . Dashed lines correspond to the inner condensate, solid lines - to outer one. From Fig.2(c) one can see that the critical velocities really can intersect. Physically this means that there is a possibility to exchange the vortex states between condensates by shifting the centers of the trapping potentials with respect to each other for fixed angular velocities.

In summary, we investigated the behaviour of simultaneously trapped condensates consisting of ^{87}Rb atoms in two different hyperfine states. It is shown that the small shift of the minima of the trapping potentials with respect to each other leads to the considerable displacement of the centers of mass of the condensates in agreement with the experiment [7]. It is also shown that the critical angular velocities of the vortex states of the condensates drastically depend on the shift and relative number of particles in the condensates. The predicted exchange of the vortex states between the condensates as a function of the shift remains to be studied experimentally.

This work is supported in part by NATO Grant No. PST.CLG.976038. V.N.R. and E.E.T. are grateful to Bartyol Research Institute of the University of Delaware for hospitality.

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Figures captions

Fig.1. Density profiles of the condensates as functions of the vertical coordinate z for $N_1 = N_2$. Figure (a) corresponds to $\alpha > \alpha_c$ and figures (b)-(c) – to $\alpha < \alpha_c$. Solid lines correspond to the $|1\rangle$ atoms and dashed lines – to the $|2\rangle$ atoms.

Fig.2. Critical velocities of outer condensate Ω_{N_1}/ω and the inner condensate Ω_{N_2}/ω as functions of α for different values of N_2/N_1 . Dashed lines correspond to Ω_{N_2}/ω and solid lines – to Ω_{N_1}/ω .

$$|\psi'(r)|^2$$



